Stochastic Multi-Objective Optimization of Heat- and Corrosion-Resistant Alloy Properties

Stochastic optimization algorithms will optimize the composition of H-series steel alloys for optimized mechanical and corrosion properties

The project will create a computational modeling tool to customize H-series alloys for specified applications and required properties. The tool will reduce or minimize the need for the addition of expensive alloying elements (including Cr, Ni, Co, Nb, Ti, V) while obtaining the optimum properties needed to design the components. This project focuses on the industry-wide need for improving materials-property performance for the applications that they are currently used for and to increase alloy upper-use temperature, thus leading to improved process efficiencies, including chemical and heat-treating processes carried out at higher temperatures than are currently used. The project takes the new approach of using stochastic optimization algorithms for optimizing H-Series steel compositions with a minimum number of experimental measurements of the composition/properties of candidate alloys. The approach has the potential of identifying new compositions that cannot be identified without carrying out hundreds of experiments. Furthermore, the approach has the potential for creating and designing alloys for specific applications, thereby maximizing their utilization at reduced cost.

Benefits

Benefits include

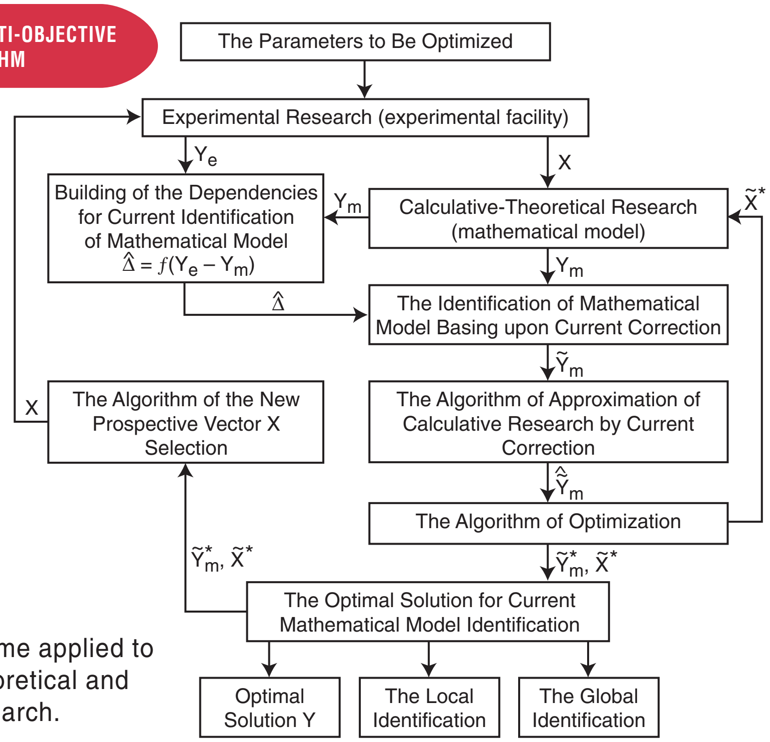
- A method to determine optimum concentrations of alloying elements in heat-resistant and corrosion-resistant H-Series austenitic stainless steel alloys that will simultaneously maximize a number of the alloy's mechanical and corrosion properties.
- A rigorous tool for the design of high-strength H-Series steels and other types of alloys unattainable by any means existing at the present time.
- Increased high-temperature strength by 50% and upper-use temperature by 30 to 60°C of H-Series of cast austenitic stainless steels.
- Improved energy efficiency through improved materials of construction.

Applications

The H-Series stainless steels have many applications as high-temperature alloys used in processing equipment in the following industries:

- **Chemical**,
- **Heat Treating**,
- **Process Heating**, and
- **Steel**.

Semi-Stochastic Multi-Objective Optimization Algorithm



The general scheme applied to calculation of theoretical and experimental research.

Project Description

Goal: The goal of the research is to develop a novel semi-stochastic constrained multi-objective optimization algorithm, to implement it in a computer code, and to validate the code against experimental data. The model is to be used for the optimization of the chemical compositions of H-Series alloys; several of the mechanical and corrosion properties of the alloys are to be simultaneously maximized or minimized. The objective is to predict the effect of varying composition on properties of H-Series stainless steel alloys.

Issues: H-Series steels have evolved over the last 80 years, and in most cases the improvements in strength have been obtained for specific applications by the addition of alloying elements based on a foundry manager's expertise. Such alloying additions generally improve strength with side effects of generating sigma and other embrittling phases. Furthermore, such alloy additions tend to work for the specific application and cannot be extrapolated for other operating conditions.

Approach: We propose to optimize the effect of a number of elements on the properties of Fe-Cr-Ni ternary. The model also requires a minimized number of alloy specimens that need to be produced and experimentally tested, thus minimizing the overall cost of automatically designing high-strength and corrosion-resistant H-Series austenitic alloys. Alloy properties of interest that will be optimized include strength (tensile and creep properties) and corrosion (high-temperature oxidation, carburization, sulfidation, and low-temperature corrosion in various solutions).
The objectives of the program will be met through the following tasks:
Task 1. Development of an initial plan of experiments.
Task 2. Analysis of the plan of experiment, identification of the objective functions, and objective constraints.
Task 3. Determination of a solution of particular optimization problems for objective constraints defined in Task 2.
Task 4. Experimental verification and identification of additional experiments needed.
Task 5. Preparation of alloys and development of tensile, creep, and corrosion data.
Task 6. Meetings and technical reports.

Potential payoff: Components fabricated from the new H-Series steels will result in improved efficiencies for chemical processing such as ethylene cracking, steel processing such as fabricating long-lasting rolls for heat-treating furnaces, and heat-treating furnaces enhanced with long-life radiant burner tubes that are capable of operation at higher temperatures.

Progress and Milestones

- Generate alloy compositions.
- Define the alloy algorithm for alloy compositions and properties.
- Determine algorithm solutions for various types of alloys and properties.
- Complete initial experiments to validate the algorithm solutions for alloy composition, strength, creep, and corrosion.
- Complete algorithm, prepare alloys, measure properties, and relate results of algorithm to experimental results.

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January 2002

ORNL 2002-01724/chj